



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:21 am GMT

PDB ID : 4AU9  
Title : Crystal Structure of a Fungal DyP-Type Peroxidase from *Auricularia auricula-judae*  
Authors : Strittmatter, E.; Pecyna, M.; Ullrich, R.; Hofrichter, M.; Plattner, D.A.; Liers, C.; Piontek, K.  
Deposited on : 2012-05-14  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

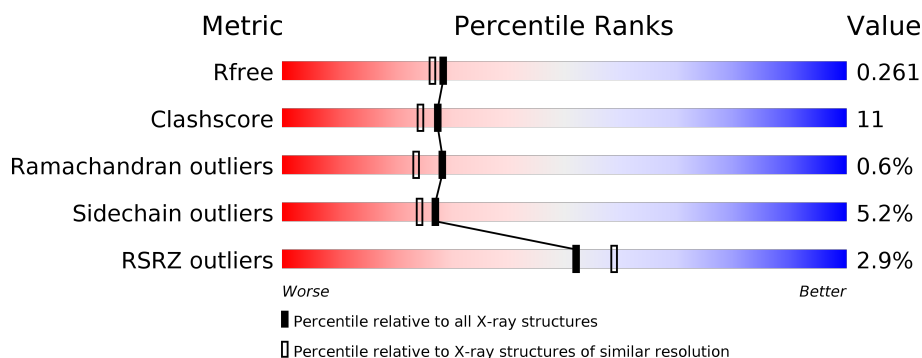
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>17%</span> </div> </div>
1	B	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 70%, grey 27%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>70%</span> <span>27%</span> </div> </div>

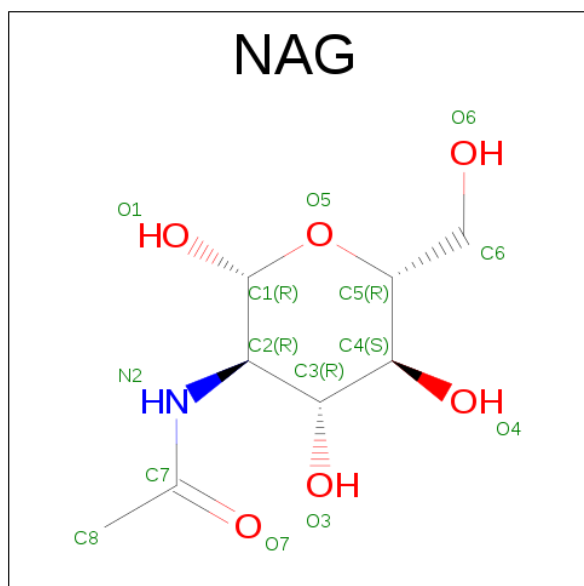
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	711	X	-	-	-
5	GOL	A	800	-	-	-	X
5	GOL	A	802	-	-	-	X
5	GOL	B	802	-	-	-	X
5	GOL	B	803	-	-	-	X
8	TAM	B	801	-	-	-	X



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

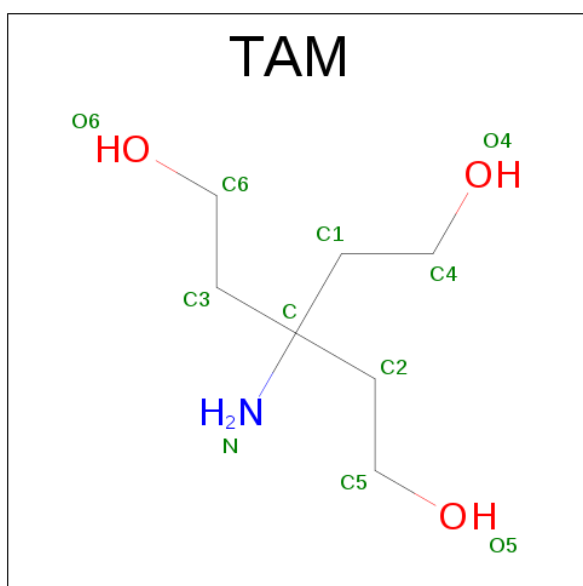


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 9 is water.

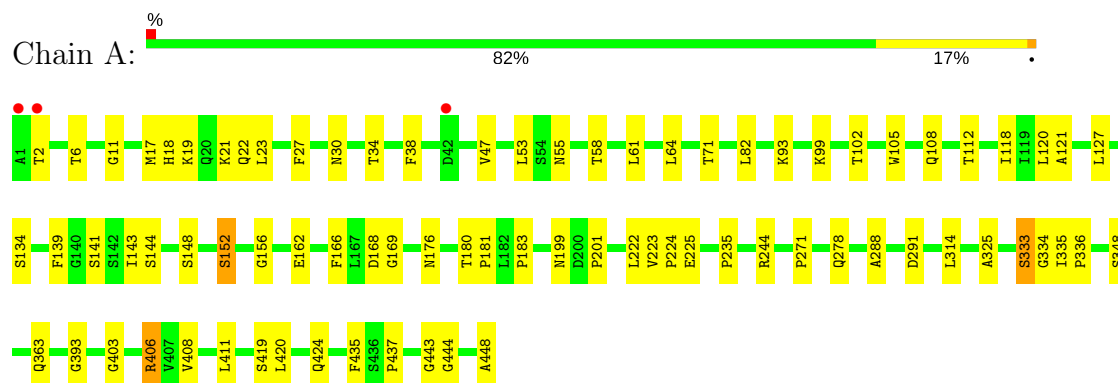
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	393	Total	O	0	0
			393	393		
9	B	286	Total	O	0	0
			286	286		



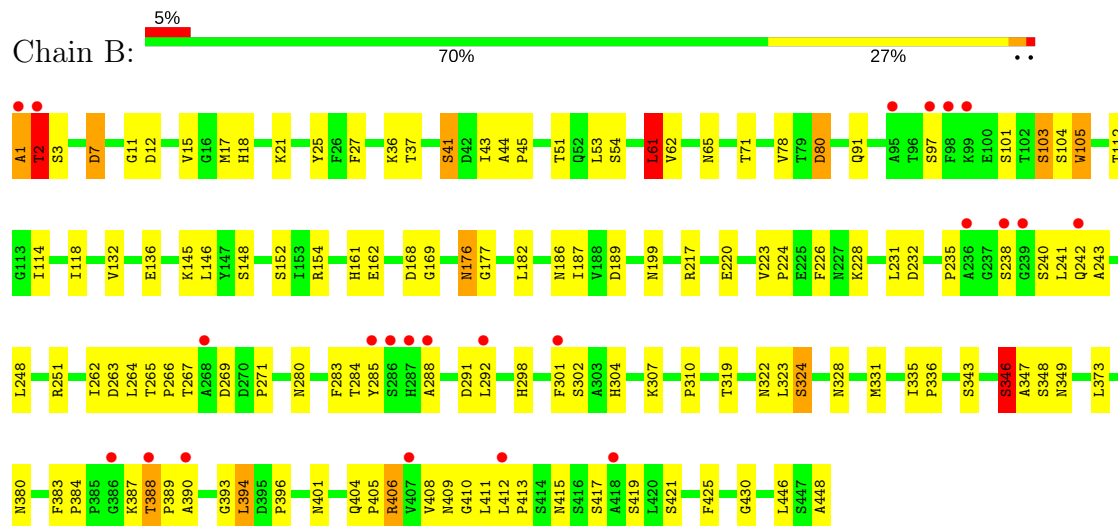
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: DYP-TYPE PEROXIDASE I



#### • Molecule 1: DYP-TYPE PEROXIDASE I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.60Å 46.69Å 141.20Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	49.03 – 2.10 49.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.03-2.10) 96.9 (49.01-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.180 , 0.261 0.181 , 0.261	Depositor DCC
$R_{free}$ test set	2483 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, TAM, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.57	0/3404	0.63	0/4644
1	B	0.48	0/3404	0.57	0/4644
All	All	0.53	0/6808	0.61	0/9288

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	ASN	Peptide
1	A	288	ALA	Peptide
1	B	1	ALA	Peptide
1	B	105	TRP	Peptide
1	B	176	ASN	Peptide
1	B	238	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3323	0	3227	51	0
1	B	3323	0	3228	96	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
3	A	39	0	34	2	0
4	A	28	0	26	1	0
4	B	14	0	13	1	0
5	A	18	0	24	3	0
5	B	18	0	24	1	0
6	A	4	0	3	0	0
7	B	28	0	25	1	0
8	B	11	0	17	3	0
9	A	393	0	0	7	0
9	B	286	0	0	18	0
All	All	7571	0	6681	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[A]:ASP:OD1	1:A:169:GLY:N	1.72	1.21
7:B:702:NAG:H2	9:B:2284:HOH:O	1.46	1.16
3:A:702:NAG:H62	3:A:703:BMA:C1	1.76	1.15
1:B:61:LEU:HD12	1:B:62:VAL:H	1.05	1.14
1:A:21:LYS:HD3	1:A:152:SER:HB3	1.36	1.03
1:B:240:SER:HB2	9:B:2195:HOH:O	1.57	1.02
1:B:168[A]:ASP:OD1	1:B:169:GLY:N	1.93	1.01
1:B:61:LEU:CD1	1:B:62:VAL:H	1.77	0.95
1:A:334:GLY:O	5:A:801:GOL:H31	1.67	0.94
1:B:61:LEU:HD12	1:B:62:VAL:N	1.83	0.91
1:B:240:SER:HB3	1:B:243:ALA:H	1.38	0.87
1:B:291:ASP:OD2	9:B:2224:HOH:O	1.95	0.82
1:B:1:ALA:HA	9:B:2001:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ASN:OD1	1:B:419:SER:OG	2.00	0.79
1:B:2:THR:HG22	1:B:3:SER:H	1.51	0.76
1:A:6:THR:H	5:A:800:GOL:H12	1.52	0.73
1:A:58:THR:HG22	1:A:58:THR:O	1.88	0.72
3:A:702:NAG:C6	3:A:703:BMA:C1	2.59	0.70
1:B:298:HIS:HB2	9:B:2228:HOH:O	1.92	0.70
1:B:189:ASP:OD2	1:B:199:ASN:ND2	2.25	0.70
1:B:25:TYR:CE2	1:B:145:LYS:HD2	2.26	0.69
1:B:408:VAL:CG2	1:B:411:LEU:HD11	2.22	0.69
1:B:322:ASN:OD1	1:B:324:SER:HB3	1.93	0.69
1:B:413:PRO:HD2	9:B:2276:HOH:O	1.93	0.69
1:B:251:ARG:NH2	1:B:410:GLY:O	2.26	0.68
1:B:408:VAL:HG22	1:B:411:LEU:HD11	1.73	0.68
1:A:271:PRO:HD2	9:A:2268:HOH:O	1.96	0.65
1:B:44:ALA:HB3	1:B:45:PRO:HD3	1.78	0.65
1:A:55:ASN:HB3	1:A:58:THR:HB	1.79	0.65
1:A:17:MET:O	1:A:18:HIS:HB2	1.97	0.65
1:A:223:VAL:HB	1:A:224:PRO:HD3	1.79	0.64
1:B:21:LYS:HD3	1:B:152:SER:HB3	1.79	0.63
1:A:444:GLY:O	1:A:448:ALA:HB3	1.98	0.63
1:A:58:THR:O	1:A:58:THR:CG2	2.45	0.63
1:B:401:ASN:HD22	1:B:404:GLN:HB2	1.64	0.61
1:B:264:LEU:HD21	1:B:283:PHE:HB3	1.83	0.60
1:B:15:VAL:O	1:B:15:VAL:HG22	2.01	0.59
1:A:19:LYS:HB2	1:A:121:ALA:HB1	1.84	0.59
1:B:251:ARG:NE	1:B:411:LEU:O	2.35	0.59
1:B:61:LEU:CG	1:B:62:VAL:H	2.14	0.59
1:B:132:VAL:O	1:B:136:GLU:HG3	2.02	0.58
1:A:333:SER:OG	5:A:802:GOL:O1	2.21	0.58
1:A:34:THR:HG22	1:A:38:PHE:HE2	1.68	0.58
1:B:12:ASP:HB2	1:B:17:MET:HE2	1.84	0.57
1:B:101:SER:OG	9:B:2088:HOH:O	2.18	0.57
1:B:11:GLY:HA3	1:B:53:LEU:HD12	1.87	0.57
1:A:102:THR:HA	1:A:105:TRP:CD1	2.40	0.57
1:B:105:TRP:CD2	1:B:430:GLY:HA3	2.39	0.57
1:A:444:GLY:O	1:A:448:ALA:CB	2.53	0.56
1:B:396:PRO:O	1:B:406:ARG:NH2	2.37	0.55
1:A:23:LEU:HD11	1:A:148:SER:OG	2.07	0.55
1:A:435:PHE:O	1:A:437:PRO:HD3	2.08	0.54
1:A:403:GLY:HA2	1:A:424:GLN:OE1	2.09	0.53
1:B:302:SER:O	1:B:396:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:THR:HG21	1:B:112:THR:HB	1.91	0.53
1:A:393:GLY:HA2	9:A:2366:HOH:O	2.08	0.52
1:B:335:ILE:HG13	1:B:336:PRO:HD2	1.91	0.52
1:B:387:LYS:O	1:B:390:ALA:HA	2.09	0.51
1:B:145:LYS:CE	1:B:148:SER:HB2	2.40	0.51
1:B:262:ILE:O	1:B:266:PRO:HB3	2.10	0.51
1:A:34:THR:HG22	1:A:38:PHE:CE2	2.45	0.51
1:B:21:LYS:HD3	1:B:152:SER:CB	2.41	0.50
1:B:388:THR:HA	1:B:389:PRO:C	2.30	0.50
1:A:143:ILE:HG13	1:A:143:ILE:O	2.12	0.50
1:A:108:GLN:OE1	1:A:108:GLN:N	2.44	0.50
1:A:348:SER:HA	4:A:711:NAG:H82	1.92	0.50
1:B:310:PRO:HD2	9:B:2232:HOH:O	2.11	0.50
1:B:176:ASN:OD1	1:B:177:GLY:N	2.45	0.49
1:B:240:SER:OG	1:B:242:GLN:HB3	2.13	0.49
1:B:145:LYS:HE3	1:B:148:SER:HB2	1.93	0.49
1:B:105:TRP:CE2	1:B:430:GLY:HA2	2.47	0.49
8:B:801:TAM:H32	8:B:801:TAM:H52	1.52	0.48
1:A:99:LYS:NZ	9:A:2101:HOH:O	2.47	0.48
1:A:199:ASN:O	1:A:201:PRO:HD3	2.14	0.47
1:A:30:ASN:HB2	1:A:141:SER:O	2.14	0.47
5:B:803:GOL:H31	9:B:2133:HOH:O	2.13	0.47
1:B:393:GLY:HA3	1:B:408:VAL:HA	1.95	0.47
1:B:269:ASP:CG	1:B:271:PRO:HD3	2.34	0.47
1:B:226:PHE:HD1	1:B:425:PHE:CD2	2.32	0.47
1:B:401:ASN:ND2	1:B:404:GLN:HB2	2.29	0.47
1:B:307:LYS:NZ	1:B:380:ASN:O	2.48	0.47
1:B:349:ASN:ND2	9:B:2250:HOH:O	2.22	0.47
1:A:64:LEU:HD12	1:A:120:LEU:HD21	1.97	0.46
1:A:61:LEU:HD21	1:A:127:LEU:HD22	1.98	0.46
1:B:15:VAL:HG22	1:B:18:HIS:NE2	2.30	0.46
1:A:93:LYS:HD2	9:A:2090:HOH:O	2.14	0.46
1:B:404:GLN:HB3	1:B:405:PRO:HD2	1.97	0.46
1:A:71:THR:HG21	1:A:112:THR:HB	1.97	0.46
1:B:103:SER:HB2	9:B:2088:HOH:O	2.16	0.46
1:B:331:MET:HE2	9:B:2014:HOH:O	2.16	0.46
1:B:348:SER:HA	4:B:711:NAG:H82	1.97	0.46
1:A:336:PRO:HD3	9:A:2164:HOH:O	2.15	0.46
1:A:443:GLY:N	9:A:2380:HOH:O	2.20	0.46
1:B:263:ASP:OD2	1:B:285:TYR:HA	2.15	0.46
1:A:11:GLY:HA3	1:A:53:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG22	1:A:64:LEU:CD2	2.47	0.45
1:A:156:GLY:N	9:A:2150:HOH:O	2.48	0.45
1:B:228:LYS:HA	1:B:231:LEU:HD12	1.99	0.45
1:B:112:THR:HG21	9:B:2084:HOH:O	2.16	0.44
1:B:15:VAL:O	1:B:15:VAL:CG2	2.64	0.44
1:B:168[B]:ASP:HA	2:B:550:HEM:HBA2	1.99	0.44
1:B:101:SER:C	1:B:103:SER:H	2.20	0.44
1:B:91:GLN:OE1	1:B:217:ARG:HD3	2.17	0.44
1:B:176:ASN:HA	1:B:177:GLY:HA2	1.87	0.44
1:B:383:PHE:CG	1:B:384:PRO:HA	2.53	0.44
1:A:21:LYS:HD3	1:A:152:SER:CB	2.26	0.44
1:A:235:PRO:O	1:A:244:ARG:HD2	2.17	0.44
1:B:168[A]:ASP:HA	2:B:550:HEM:HBA2	2.00	0.44
1:A:223:VAL:N	1:A:224:PRO:HD2	2.33	0.43
1:A:223:VAL:N	1:A:224:PRO:CD	2.80	0.43
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.83	0.43
1:B:145:LYS:HE3	9:B:2130:HOH:O	2.17	0.43
1:B:186:ASN:OD1	1:B:187:ILE:N	2.51	0.43
1:B:145:LYS:CE	1:B:148:SER:CB	2.97	0.43
1:A:411:LEU:HD12	1:A:420:LEU:HD12	2.01	0.43
1:A:314:LEU:HD12	1:A:325:ALA:HB2	2.01	0.43
1:B:27:PHE:CE2	1:B:118:ILE:HG13	2.53	0.43
1:B:304:HIS:CD2	2:B:550:HEM:NA	2.87	0.43
1:B:389:PRO:HD2	9:B:2227:HOH:O	2.19	0.43
1:A:162:GLU:HG3	1:A:166:PHE:O	2.19	0.43
1:B:412:LEU:HA	1:B:413:PRO:HD3	1.94	0.43
1:B:80:ASP:N	1:B:80:ASP:OD1	2.43	0.43
1:B:220:GLU:HG3	9:B:2184:HOH:O	2.19	0.43
1:B:223:VAL:HB	1:B:224:PRO:CD	2.48	0.43
1:B:43:ILE:O	1:B:44:ALA:C	2.58	0.42
1:B:7:ASP:OD1	1:B:51:THR:OG1	2.25	0.42
1:A:139:PHE:HB3	1:A:143:ILE:HG12	2.00	0.42
1:A:335:ILE:HA	1:A:336:PRO:HD3	1.87	0.42
1:B:346:SER:O	1:B:348:SER:N	2.51	0.42
1:A:180:THR:HA	1:A:181:PRO:HD3	1.84	0.42
1:B:284:THR:O	1:B:285:TYR:HB2	2.20	0.42
1:B:322:ASN:O	1:B:323:LEU:HD23	2.20	0.42
1:A:27:PHE:CE2	1:A:118:ILE:HG13	2.55	0.42
1:B:37:THR:O	1:B:41:SER:HB2	2.19	0.42
1:A:22:GLN:HA	1:A:120:LEU:O	2.19	0.42
1:B:154:ARG:NH2	9:B:2139:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:PRO:HD3	1:B:248:LEU:HB2	2.02	0.41
1:B:61:LEU:CG	1:B:62:VAL:N	2.81	0.41
1:A:183:PRO:HG2	1:A:278:GLN:O	2.20	0.41
1:B:161:HIS:CD2	1:B:161:HIS:N	2.88	0.41
1:B:36:LYS:NZ	1:B:448:ALA:O	2.41	0.41
1:A:222:LEU:HB3	1:A:225:GLU:OE1	2.20	0.41
1:B:228:LYS:HE3	1:B:232:ASP:OD2	2.20	0.41
1:B:328:ASN:O	1:B:373:LEU:HD11	2.21	0.41
1:B:415:ASN:ND2	9:B:2277:HOH:O	2.52	0.41
1:B:78:VAL:HG21	1:B:446:LEU:HD23	2.03	0.41
1:B:396:PRO:O	1:B:406:ARG:NH1	2.49	0.41
8:B:801:TAM:HN1	8:B:801:TAM:H41	1.59	0.41
1:B:394:LEU:HD13	8:B:801:TAM:H61	2.03	0.40
1:B:114:ILE:HG13	1:B:146:LEU:HD12	2.04	0.40
1:B:1:ALA:C	1:B:2:THR:OG1	2.60	0.40
1:B:301:PHE:CE1	1:B:387:LYS:HD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/448 (100%)	431 (96%)	16 (4%)	0	100	100
1	B	447/448 (100%)	417 (93%)	25 (6%)	5 (1%)	17	11
All	All	894/896 (100%)	848 (95%)	41 (5%)	5 (1%)	28	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	288	ALA
1	B	346	SER
1	B	347	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/354 (100%)	344 (97%)	11 (3%)	45	48
1	B	355/354 (100%)	329 (93%)	26 (7%)	16	13
All	All	710/708 (100%)	673 (95%)	37 (5%)	27	24

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	82	LEU
1	A	134	SER
1	A	144	SER
1	A	152	SER
1	A	291	ASP
1	A	333	SER
1	A	363	GLN
1	A	406	ARG
1	A	408	VAL
1	A	419	SER
1	B	2	THR
1	B	7	ASP
1	B	41	SER
1	B	54	SER
1	B	61	LEU
1	B	65	ASN
1	B	80	ASP
1	B	97	SER
1	B	103	SER

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Mol	Chain	Res	Type
1	B	104	SER
1	B	162	GLU
1	B	182	LEU
1	B	241	LEU
1	B	265	THR
1	B	267	THR
1	B	280	ASN
1	B	292	LEU
1	B	319	THR
1	B	324	SER
1	B	343	SER
1	B	346	SER
1	B	388	THR
1	B	394	LEU
1	B	406	ARG
1	B	417	SER
1	B	421	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	199	ASN
1	A	233	ASN
1	A	242	GLN
1	A	382	ASN
1	B	233	ASN
1	B	242	GLN
1	B	280	ASN
1	B	298	HIS
1	B	375	GLN
1	B	401	ASN
1	B	402	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

5 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	701	1,3	14,14,15	0.63	0	15,19,21	1.29	2 (13%)
3	NAG	A	702	3	14,14,15	0.62	0	15,19,21	0.97	0
3	BMA	A	703	3	11,11,12	0.52	0	13,15,17	1.03	1 (7%)
7	NAG	B	701	1,7	14,14,15	0.50	0	15,19,21	1.04	1 (6%)
7	NAG	B	702	7	14,14,15	0.63	0	15,19,21	1.10	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	-	0/6/23/26	0/1/1/1
3	BMA	A	703	3	-	0/2/19/22	1/1/1/1
7	NAG	B	701	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	702	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	O5-C1-C2	-3.17	107.06	111.47
7	B	701	NAG	O5-C1-C2	-3.04	107.25	111.47
7	B	702	NAG	C1-O5-C5	-2.49	108.73	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	C2-N2-C7	-2.16	119.80	122.94
7	B	702	NAG	C4-C3-C2	2.47	114.63	111.02
3	A	703	BMA	C1-O5-C5	2.84	116.08	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAG	2	0
3	A	703	BMA	2	0
7	B	702	NAG	1	0

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	HEM	A	550	1	28,50,50	2.09	7 (25%)	17,82,82	1.53	5 (29%)
4	NAG	A	711	1	14,14,15	0.49	0	15,19,21	0.89	0
4	NAG	A	721	1	14,14,15	0.61	0	15,19,21	1.35	3 (20%)
5	GOL	A	800	-	5,5,5	0.37	0	5,5,5	0.18	0
5	GOL	A	801	-	5,5,5	0.34	0	5,5,5	0.25	0
5	GOL	A	802	-	5,5,5	0.24	0	5,5,5	0.45	0
6	ACT	A	803	-	1,3,3	1.35	0	0,3,3	0.00	-
2	HEM	B	550	1	28,50,50	2.33	10 (35%)	17,82,82	1.91	4 (23%)
4	NAG	B	711	1	14,14,15	0.71	0	15,19,21	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	800	-	5,5,5	0.37	0	5,5,5	0.33	0
8	TAM	B	801	-	7,10,10	0.51	0	9,12,12	0.44	0
5	GOL	B	802	-	5,5,5	0.33	0	5,5,5	0.15	0
5	GOL	B	803	-	5,5,5	0.31	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	550	1	-	0/6/54/54	0/0/8/8
4	NAG	A	711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	721	1	-	0/6/23/26	0/1/1/1
5	GOL	A	800	-	-	0/4/4/4	0/0/0/0
5	GOL	A	801	-	-	0/4/4/4	0/0/0/0
5	GOL	A	802	-	-	0/4/4/4	0/0/0/0
6	ACT	A	803	-	-	0/0/0/0	0/0/0/0
2	HEM	B	550	1	-	0/6/54/54	0/0/8/8
4	NAG	B	711	1	1/1/5/7	0/6/23/26	0/1/1/1
5	GOL	B	800	-	-	0/4/4/4	0/0/0/0
8	TAM	B	801	-	-	0/12/12/12	0/0/0/0
5	GOL	B	802	-	-	0/4/4/4	0/0/0/0
5	GOL	B	803	-	-	0/4/4/4	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	550	HEM	C3C-C2C	-4.65	1.34	1.40
2	B	550	HEM	C3B-C2B	-4.62	1.34	1.40
2	A	550	HEM	C3B-C2B	-3.80	1.35	1.40
2	A	550	HEM	C3C-C2C	-3.52	1.35	1.40
2	B	550	HEM	CAA-C2A	2.12	1.55	1.52
2	B	550	HEM	CMC-C2C	2.13	1.56	1.51
2	B	550	HEM	C4A-NA	2.14	1.40	1.36
2	A	550	HEM	CAA-C2A	2.29	1.55	1.52
2	B	550	HEM	C4C-NC	2.73	1.40	1.36
2	A	550	HEM	C4D-ND	2.93	1.40	1.36
2	B	550	HEM	C3B-CAB	2.95	1.53	1.47
2	B	550	HEM	C3C-CAC	3.58	1.54	1.47
2	A	550	HEM	C3C-CAC	3.67	1.55	1.47
2	B	550	HEM	C4D-ND	4.03	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	HEM	C3B-CAB	4.18	1.56	1.47
2	A	550	HEM	C3D-C2D	4.86	1.52	1.37
2	B	550	HEM	C3D-C2D	5.04	1.52	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	HEM	CAA-CBA-CGA	-4.12	105.62	112.66
4	A	721	NAG	C2-N2-C7	-3.15	118.35	122.94
2	B	550	HEM	CAD-CBD-CGD	-3.05	107.45	112.66
2	A	550	HEM	CAD-CBD-CGD	-2.63	108.16	112.66
2	A	550	HEM	CBA-CAA-C2A	-2.41	107.87	112.48
2	A	550	HEM	CBD-CAD-C3D	-2.36	107.97	112.47
4	A	721	NAG	O3-C3-C4	-2.35	105.25	110.36
2	A	550	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
4	A	721	NAG	O5-C1-C2	-2.07	108.60	111.47
2	B	550	HEM	CMD-C2D-C1D	2.34	132.06	128.46
2	A	550	HEM	CMB-C2B-C3B	2.37	129.29	124.89
4	B	711	NAG	C4-C3-C2	2.39	114.52	111.02
2	B	550	HEM	C4A-C3A-C2A	2.80	108.94	107.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	711	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	711	NAG	1	0
5	A	800	GOL	1	0
5	A	801	GOL	1	0
5	A	802	GOL	1	0
2	B	550	HEM	3	0
4	B	711	NAG	1	0
8	B	801	TAM	3	0
5	B	803	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	448/448 (100%)	-0.25	3 (0%) 87 89	5, 19, 33, 65	0
1	B	448/448 (100%)	0.21	23 (5%) 29 35	10, 28, 51, 68	0
All	All	896/896 (100%)	-0.02	26 (2%) 52 59	5, 22, 46, 68	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.8
1	B	1	ALA	6.5
1	A	1	ALA	4.9
1	A	2	THR	3.6
1	B	98	PHE	3.4
1	B	99	LYS	3.4
1	B	288	ALA	3.4
1	B	412	LEU	3.0
1	B	268	ALA	3.0
1	B	285	TYR	3.0
1	B	238	SER	3.0
1	B	386	GLY	2.9
1	B	390	ALA	2.8
1	B	236	ALA	2.6
1	B	242	GLN	2.4
1	B	388	THR	2.4
1	B	97	SER	2.4
1	B	407	VAL	2.3
1	B	292	LEU	2.3
1	A	42	ASP	2.3
1	B	239	GLY	2.3
1	B	287	HIS	2.2
1	B	418	ALA	2.2
1	B	286	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	2.2
1	B	301	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	702	14/15	0.78	0.21	-	42,45,50,51	0
3	BMA	A	703	11/12	0.48	0.35	-	53,55,56,57	0
7	NAG	B	701	14/15	0.84	0.25	-	54,57,60,62	0
7	NAG	B	702	14/15	0.62	0.39	-	63,67,68,68	0
3	NAG	A	701	14/15	0.90	0.12	-	27,33,36,41	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	803	6/6	0.71	0.23	7.57	47,48,49,49	0
5	GOL	A	802	6/6	0.83	0.22	7.01	48,49,51,51	0
5	GOL	B	802	6/6	0.68	0.25	6.59	59,60,61,61	0
8	TAM	B	801	11/11	0.73	0.29	2.54	53,54,56,56	0
5	GOL	A	800	6/6	0.83	0.19	2.09	46,47,48,48	0
5	GOL	B	800	6/6	0.91	0.17	1.99	57,58,58,59	0
4	NAG	B	711	14/15	0.78	0.24	1.68	44,48,50,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	721	14/15	0.92	0.14	0.49	19,26,29,30	0
4	NAG	A	711	14/15	0.94	0.12	0.38	27,30,32,34	0
5	GOL	A	801	6/6	0.79	0.15	0.36	51,52,52,53	0
2	HEM	B	550	43/43	0.97	0.12	-0.18	10,17,26,28	0
2	HEM	A	550	43/43	0.98	0.10	-0.22	3,8,13,14	0
6	ACT	A	803	4/4	0.79	0.19	-	67,67,67,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.